

XP-002327913

Substance Identification

Beilstein Registry Number

Beilstein Preferred RN 101172-52-5 CAS Registry Number 101172-52-5

Chemical Name 6-hydroxy-2-methyl-octahydro-isoquinoline-8a-carboxylic acid

ethyl ester

Autoname 6-hydroxy-2-methyl-octahydro-isoquinoline-8a-carboxylic acid

ethyl ester

Molecular Formula C13H23NO3 Molecular Weight 241.33

Lawson Number 26671, 2817, 298

Type of Substance heterocyclic Constitution ID 175870 127683

Beilstein Reference 4-22-00-02111 Entry Date 1988/06/27 Update Date 1992/05/13

Field Availability List 1-3 of 3

Code	Field Name	Occ
	Reaction Boiling Point Reference	3 1 1
14.4		

Reaction 1 of 3

Reaction ID

Reactant BRN

186484 6-hydroxy-2-methyl-octahydro-isoquinoline-8a-

carboxylic acid ethyl ester

Product BRN 7-methyl-hexahydro-3,8a-ethano-pyrano[3,4-c]pyridin-

1-one

No. of Reaction Details 1

Reaction Entry Date 1988/06/27 Reaction Update Date 1988/06/27

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BNSDOCID: <XP_____2327913A__I_>

eaction Classification eagent

Preparation

HCI

ntry Date

benzene 1988/06/27

lote 1

Handbook

lef. 1

; 1988/06/27; Journal; Sugimoto et al.; YKKZAJ; Yakugaku Zasshi; 75; 1955; 177; Chem.Abstr.; 1956; 1814.

Reaction 2 of 3

Reaction ID Reactant BRN

Product BRN

186484 6-hydroxy-2-methyl-octahydro-isoquinoline-8a-

carboxylic acid ethyl ester

2-methyl-6-oxo-octahydro-isoquinoline-8a-carboxylic

acid ethyl ester

No. of Reaction Details

Reaction Entry Date Reaction Update Date Reaction Classification

Reagent

Entry Date

Note 1 Ref. 1

1988/06/27

1988/06/27 Preparation

MnO₂

petroleum ether 1988/06/27

Handbook

2005 12; 1988/06/27; Journal; Sugimoto et al.; YKKZAJ; Yakugaku Zasshi; 75; 1955; 177; Chem.Abstr.; 1956; 1814.

Reaction 3 of 3

Reaction ID Reactant

(+-)-2-methyl-6-oxo-2,3,4,6,7,8-hexahydro-1*H*-isoquinoline-8a-carboxylic acid ethyl ester 6-hydroxy-2-methyl-octahydro-isoquinoline-8a-

carboxylic acid ethyl ester

Product BRN

No. of Reaction Details **Reaction Entry Date Reaction Update Date**

Reaction Classification

Reagent

1988/06/27 1988/06/27

Preparation (half reaction)

platinum ethanol

Other Conditions Entry Date

Hydrogenation 1988/06/27

Note 1 Ref. 1

Handbook

; 1988/06/27; Journal; Sugimoto et al.; YKKZAJ; Yakugaku Zasshi; 75; 1955; 177; Chem.Abstr.; 1956; 1814.

Boiling Point

VALUE (BP)

Pressure (.P)

Entry Date

Note Ref.

1

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1988/06/27

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Note 1 Ref. 1 Handbook

; 1988/06/27; Journal; Sugimoto et al.; YKKZAJ; Yakugaku Zasshi; 75; 1955; 177; Chem.Abstr.; 1956; 1814.

Reference

; 1988/06/27; Journal; Sugimoto et al.; YKKZAJ; Yakugaku Zasshi; 75; 1955; 177; Chem.Abstr.; 1956; 1814.

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